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4-(3-Methylbenzenesulfonamido)phenyl 3-methylbenzenesulfonate

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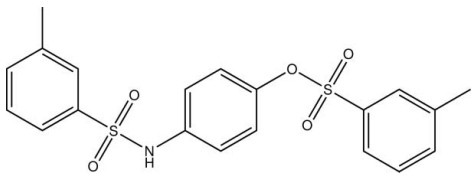
Key indicators: single-crystal X-ray study; T = 100 K; mean σ(C–C) = 0.001 Å; disorder in main residue; R factor = 0.031; wR factor = 0.090; data-to-parameter ratio = 27.6.

The complete molecule of the title compound, $C_{20}H_{19}NO_5S_2$, is generated by a crystallographic twofold axis and the O atom and N—H group attached to the central benzene ring are statistically disordered. The dihedral angle between the central and terminal benzene rings is 56.91 (5)° and that between the terminal benzene rings is 29.80 (5)°. In the crystal, N—H···O hydrogen bonding links the molecules into sheets lying parallel to the *ab* plane.

Related literature

For the biological properties of sulfonyl derivatives, see: Supuran *et al.* (2003). For a related structure, see: Sinha *et al.* (2011). For the stability of the temperature controller used in the data collection, see: Cosier & Glazer (1986).



Experimental

Crystal data

$C_{20}H_{19}NO_5S_2$
M_r = 417.48
Monoclinic, $C2/c$
a = 14.4352 (1) Å
b = 9.1250 (1) Å
c = 15.4402 (2) Å
β = 109.700 (1)°
V = 1914.76 (4) Å^3
Z = 4
Mo $K\alpha$ radiation
μ = 0.31 mm^{-1}
T = 100 K
0.41 × 0.34 × 0.25 mm

Data collection

Bruker SMART APEXII CCD diffractometer
Absorption correction: multi-scan (*SADABS*; Bruker, 2009)
T_{min} = 0.883, T_{max} = 0.926
21937 measured reflections
3533 independent reflections
3249 reflections with $I > 2\sigma(I)$
R_{int} = 0.022

Refinement

$R[F^2 > 2\sigma(F^2)]$ = 0.031
$wR(F^2)$ = 0.090
S = 1.08
3533 reflections
128 parameters
H-atom parameters constrained
$\Delta\rho_{max}$ = 0.46 e Å^{-3}
$\Delta\rho_{min}$ = −0.40 e Å^{-3}

Table 1
Hydrogen-bond geometry (Å, °).

D—H···A	D—H	H···A	D···A	D—H···A
N1—H1···O3^{i}	1.02	1.97	2.9854 (11)	178

Symmetry code: (i) $-x+\frac{1}{2}, y-\frac{1}{2}, -z+\frac{3}{2}$.

Data collection: *APEX2* (Bruker, 2009); cell refinement: *SAINT* (Bruker, 2009); data reduction: *SAINT*; program(s) used to solve structure: *SHELXTL* (Sheldrick, 2008); program(s) used to refine structure: *SHELXTL*; molecular graphics: *SHELXTL*; software used to prepare material for publication: *SHELXTL* and *PLATON* (Spek, 2009).

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Supplementary data and figures for this paper are available from the IUCr electronic archives (Reference: HB6544).

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